Angelyl Angelate

Inchi: InChI=1S/C10H16O2/c1-5-8(3)7-12-10(11)9(4)6-2/h5-6H,7H2,1-4H3/b8-5-,9-6-
InchiKey: QJXVZKLQKPUDPW-VVRUXRSYSA-N
Formula: C10H16O2
SMILES: CC=C(C)COC(=O)C(C)=CC
Mol. weight [g/mol]: 168.23

Physical Properties

Property code	Value	Unit	Source
gf	-57.26	kJ/mol	Joback Method
hf	-279.67	kJ/mol	Joback Method
hfus	22.23	kJ/mol	Joback Method
hvap	47.09	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	2.462		Crippen Method
mcvol	150.600	ml/mol	McGowan Method
pc	2455.60	kPa	Joback Method
rinpol	1199.00		NIST Webbook
tb	512.57	K	Joback Method
tc	707.11	K	Joback Method
tf	236.54	K	Joback Method
vc	0.582	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.83	J/mol×K	512.57	Joback Method
cpg	346.67	J/mol×K	544.99	Joback Method
cpg	359.82	J/mol×K	577.42	Joback Method
cpg	372.30	J/mol×K	609.84	Joback Method
cpg	384.14	J/mol×K	642.27	Joback Method
cpg	395.38	J/mol×K	674.69	Joback Method
cpg	406.04	J/mol×K	707.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R438436&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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